Data Splitting and Resampling

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Week 3, Class 1

Data Specialist at PSI

- The Data Science Specialist works with PSI scientists on various federal grants and sponsored projects, including a large-scale, multi-site center grant (P50) and the RADx-UP grant to scale-up COVID-19 testing to the Latinx community.

- The incumbent interfaces with and provides support across projects to facilitate data harmonization of projects involving multiple sources of data and means of data collection (observation, biospecimen, imaging, Qualtrics, REDCap, etc.).

- Support for other projects includes acting as a resource to personnel accessing data; coordinating with methodologists; running routine descriptive analysis; cleaning, formatting, and preparing files for datasets; and conducting light analysis, such as descriptive analysis and frequencies.

- Although remote work is possible at the start of this position, the ideal candidate would eventually be able to work on-site.

https://careers.uoregon.edu/en-us/job/525722/pro-tem-research-assistant-data-science-specialist

Agenda

- Data splitting and why it matters
- Introduce resampling methods

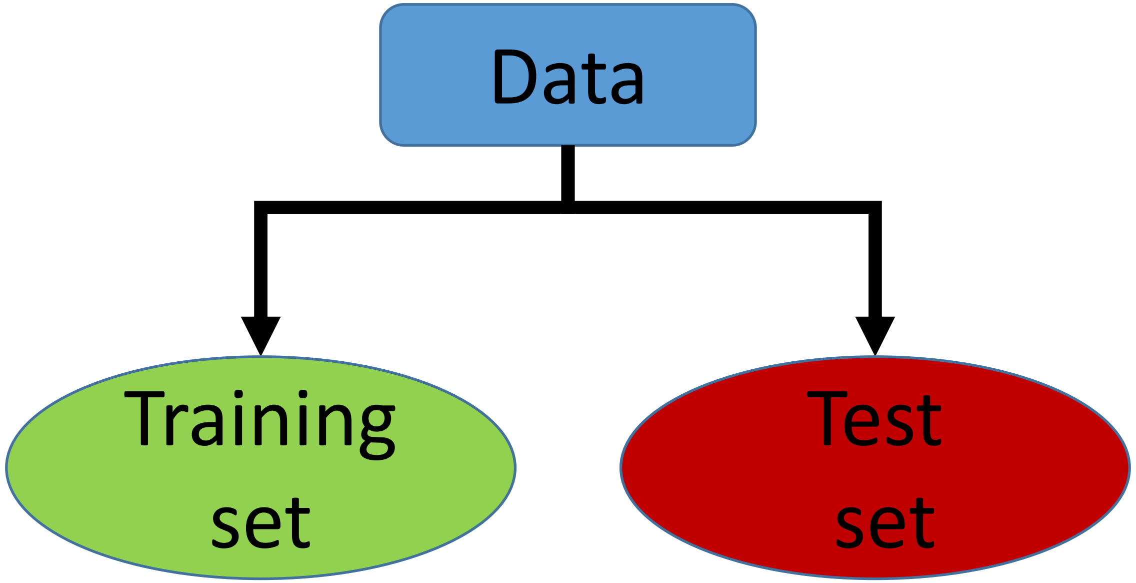
Data Splitting

Data splitting

- The goal of machine learning is to predict results based on new (unseen) data
- “The best way to measure a model's performance at predicting new data is to predict new data.” – paraphrasing/quoting multiple experts
- The simplest way to do this is to split our data into two parts:
  - **Training set**
  - **Test set**
- We then fit a model to the training data and predict the results of the test set
  - fit -> training
  - predict -> test

Data splitting

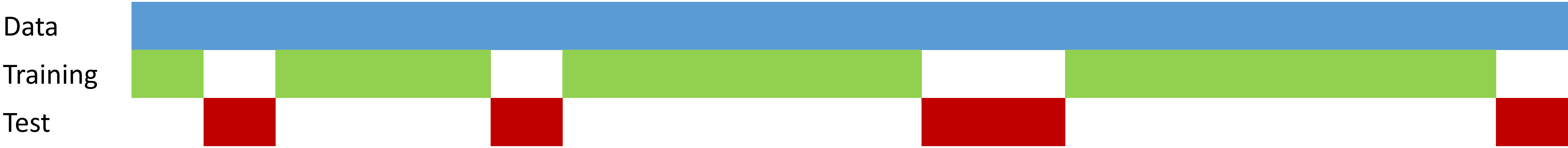
- We can do anything we want to the training set
    - train our algorithms, tune hyperparameters, compare models, and all of the other activities required to choose a final model
- We do **nothing** with the test set until we have finalized our model using from the training set
    - **Data leakage** is using ANY part of the test set in our training set
        - Using the test set during our modeling process
        - Pre-processing or feature engineering the full data (training and test sets together)
        - Time series design, when the outcome of one series is used in the prediction of the next



Data

Training set

Test set

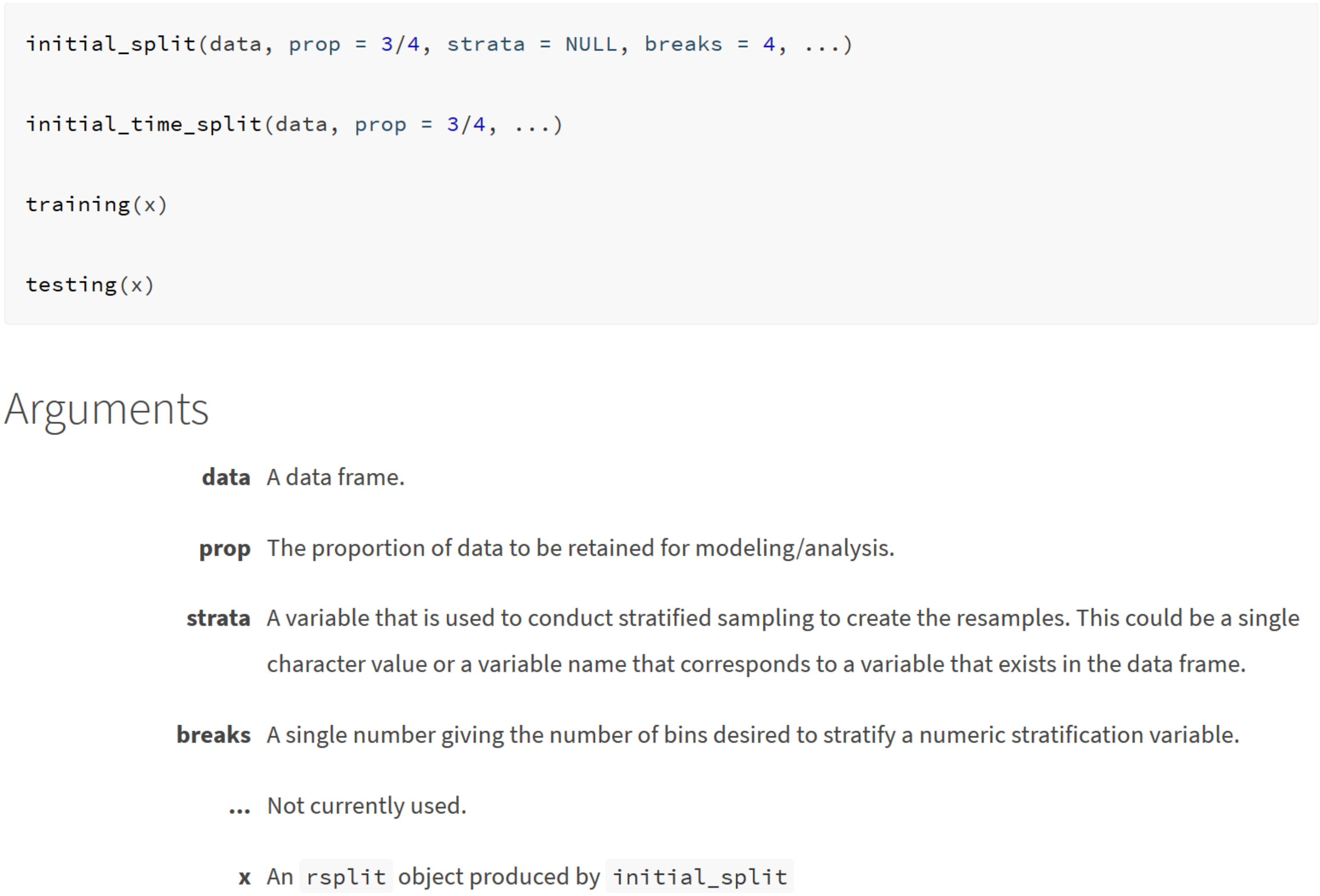


{rsample}

```
math_split <- initial_split(math)

math_train <- training(math_split)
math_test  <- testing(math_split)
```

- These three functions are meant to be used in conjunction
- A good rule is to make these the first lines of your ML project code
  - some differ

`initial_split()` help documentation



```
initial_split(data, prop = 3/4, strata = NULL, breaks = 4, ...)

initial_time_split(data, prop = 3/4, ...)

training(x)

testing(x)
```

Arguments

data A data frame.

prop The proportion of data to be retained for modeling/analysis.

strata A variable that is used to conduct stratified sampling to create the resamples. This could be a single character value or a variable name that corresponds to a variable that exists in the data frame.

breaks A single number giving the number of bins desired to stratify a numeric stratification variable.

... Not currently used.

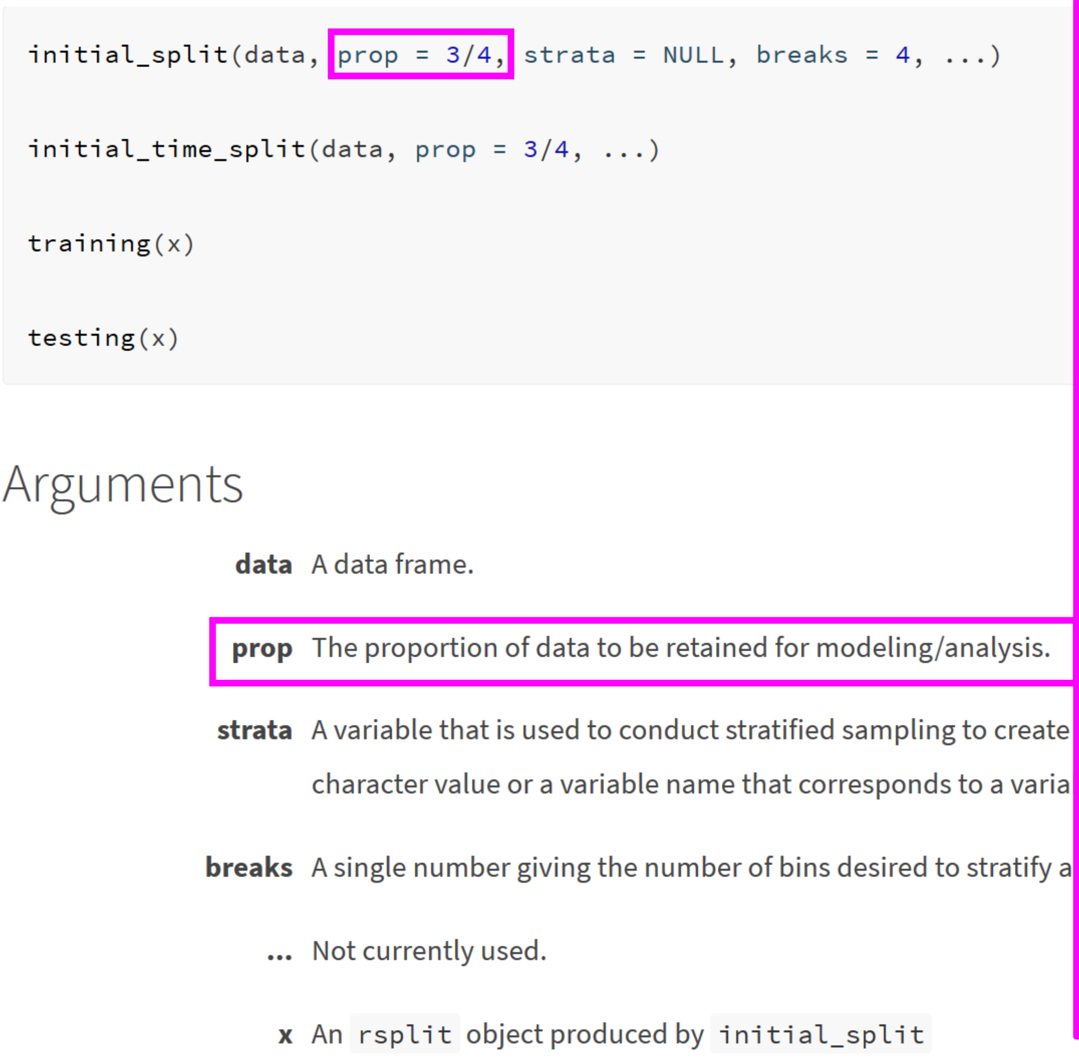
x An `rsplit` object produced by `initial_split`

Let’s take a look at initial_split()

follow along if you can

```
math <- read_csv(here::here("data", "train.csv"))

set.seed(3000)
(math_split <- initial_split(math))
<Analysis/Assess/Total>
<142070/47356/189426>

math_split %>% training() %>% nrow() / nrow(math)
[1] 0.7500026

names(math_split)
[1] "data"   "in_id"  "out_id" "id"

class(math_split)
[1] "rsplit"   "mc_split"
```

Additional arguments



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initial_split(data, prop = 3/4, strata = NULL, breaks = 4, ...)

initial_time_split(data, prop = 3/4, ...)

training(x)

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The default is simple random assignment, with:

- 75% to the training set, and
- 25% to the test set

A general guideline is somewhere between 60%/40% & 80%/20%.

- Spending too much in training (e.g., > 80%) may mean poor predictive performance. It may fit the training data very well, but is not generalizable (overfitting).
- Spending too much in testing (e.g., > 40%) may mean poor assessment of model parameters (underfitting).

- If you have a lot of data, you may see little predictive benefit of using the entire data, but an increase in computational time.
- If you have more features/predictors than rows, you may need a larger sample size to identify consistent signals in the features.

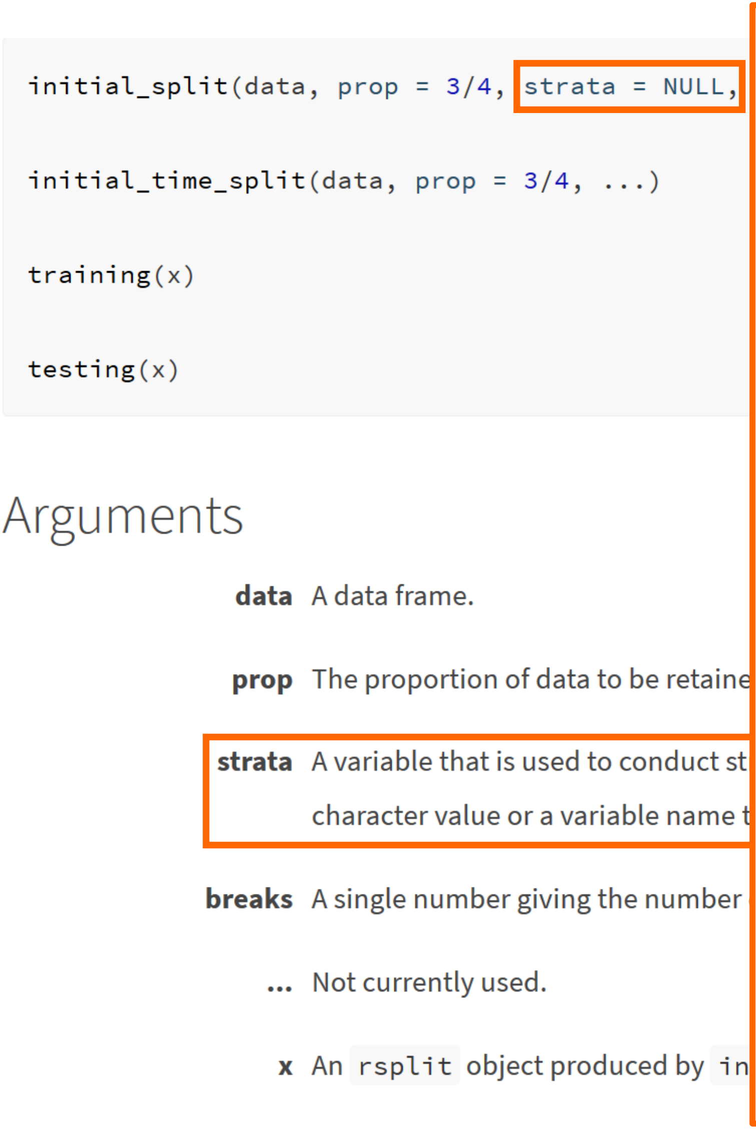
```
split_data <- initial_split(ames, prop = .70)
```

Let’s take a look at `prop`

```
set.seed(3000)
(math_split70 <- initial_split(math, prop = .70))
<Analysis/Assess/Total>
<132599/56827/189426>

math_split70 %>% training() %>% nrow() / nrow(math)
[1] 0.7000042
```

Additional arguments



```
initial_split(data, prop = 3/4, strata = NULL,

initial_time_split(data, prop = 3/4, ...)

training(x)

testing(x)
```

Arguments

data A data frame.

prop The proportion of data to be retaine

strata A variable that is used to conduct st character value or a variable name t

breaks A single number giving the number

... Not currently used.

x An `rsplit` object produced by `in`

As opposed to simple random assignment, you can use **stratified sampling** to ensure the training and test sets have similar outcome (*Y*) distributions/proportions (equal to that of the full data set). Helps ensure a balanced representation of the response distribution in both the training and test sets.

Especially useful if:

- the continuous outcome is not normally distributed (skewed)
  - stratified sampling will segment outcome into quantiles and randomly sample from each
- the categorical outcome has substantial unbalanced classes (e.g., 6% HS dropout, 94% graduate)
  - this will matter less with large data

```
split_data <- initial_split(ames, strata = Sales_Price)
```

Let’s take a look at `strata`

- Here we’re stratifying by a predictor and not the outcome

```
math_split %>%
  training() %>%
  janitor::tabyl(ethnic_cd)
 ethnic_cd     n    percent
         A  5885 0.04142324
         B  3148 0.02215809
         H 34537 0.24309847
         I  1848 0.01300767
         M  8930 0.06285634
         P  1077 0.00758077
         W 86645 0.60987541
```

```
math_split %>%
  testing() %>%
  janitor::tabyl(ethnic_cd)
 ethnic_cd     n     percent
         A  1810 0.038221134
         B  1002 0.021158882
         H 11345 0.239568376
         I   594 0.012543289
         M  2965 0.062610862
         P   353 0.007454177
         W 29287 0.618443281
```

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         P   353 0.007454177
         W 29287 0.618443281
```

```
math_split_strat <- initial_split(math, strata = ethnic_cd)
```

```
math_split_strat %>%
  training() %>%
  janitor::tabyl(ethnic_cd)
 ethnic_cd     n     percent
         A  5718 0.040247765
         B  3114 0.021918772
         H 34465 0.242591680
         I  1841 0.012958401
         M  8910 0.062715563
         P  1067 0.007510382
         W 86955 0.612057436
```

```
math_split_strat %>%
  testing() %>%
  janitor::tabyl(ethnic_cd)
 ethnic_cd     n     percent
         A  1977 0.041747614
         B  1036 0.021876848
         H 11417 0.241088774
         I   601 0.012691106
         M  2985 0.063033195
         P   363 0.007665343
         W 28977 0.611897120
```

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 ethnic_cd     n     percent
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```
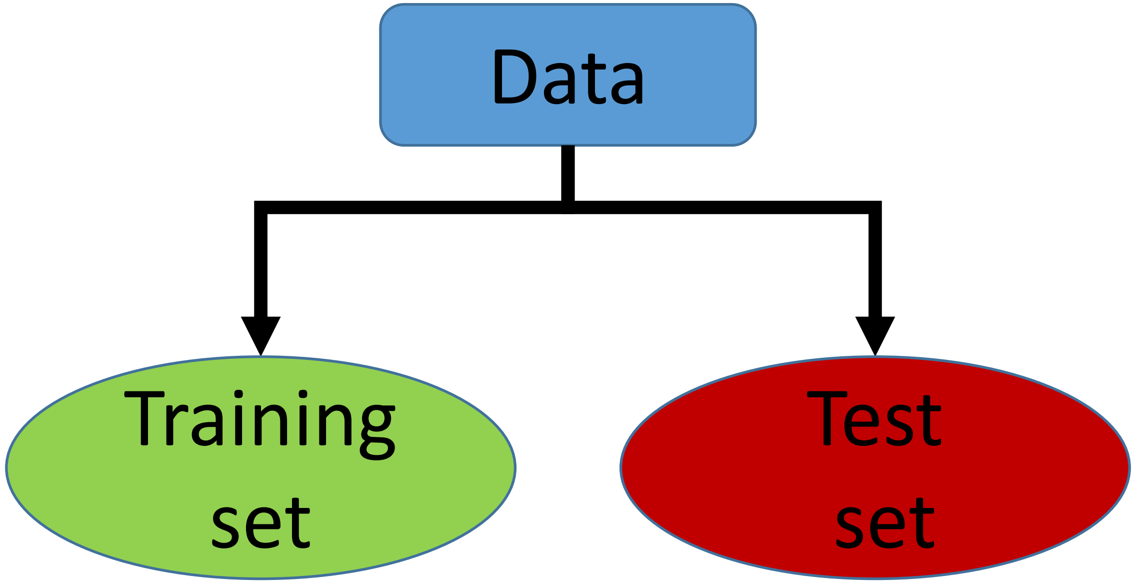

Resampling

We split – now what?

- Again, we NEVER use the test set until we have a “final model”
- And “the best way to measure a model's performance at predicting new data is to predict new data”
- So how do we measure model performance during the training phase? What new data do we predict?
- Just re-predicting the training set is not ideal
  - biases results - may well predict training set but won’t generalize to new data
  - no measure of variance if we only have one measure of performance (based on predicting the training set)
- We **resample** training set



Data

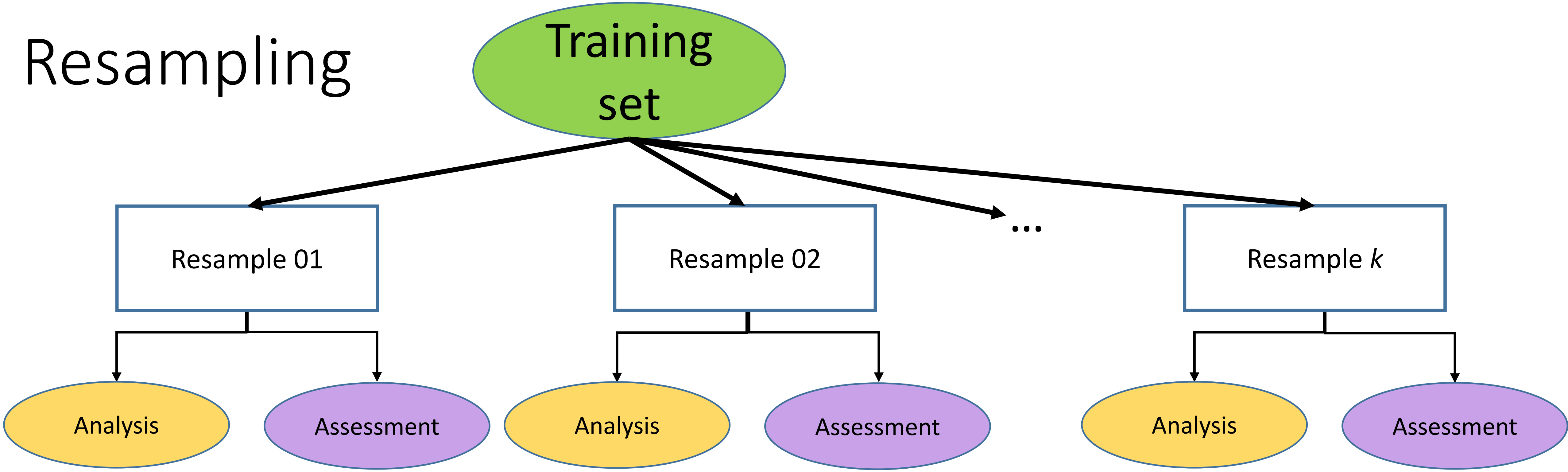
Training set

Test set

Resampling

Training set

Resampling



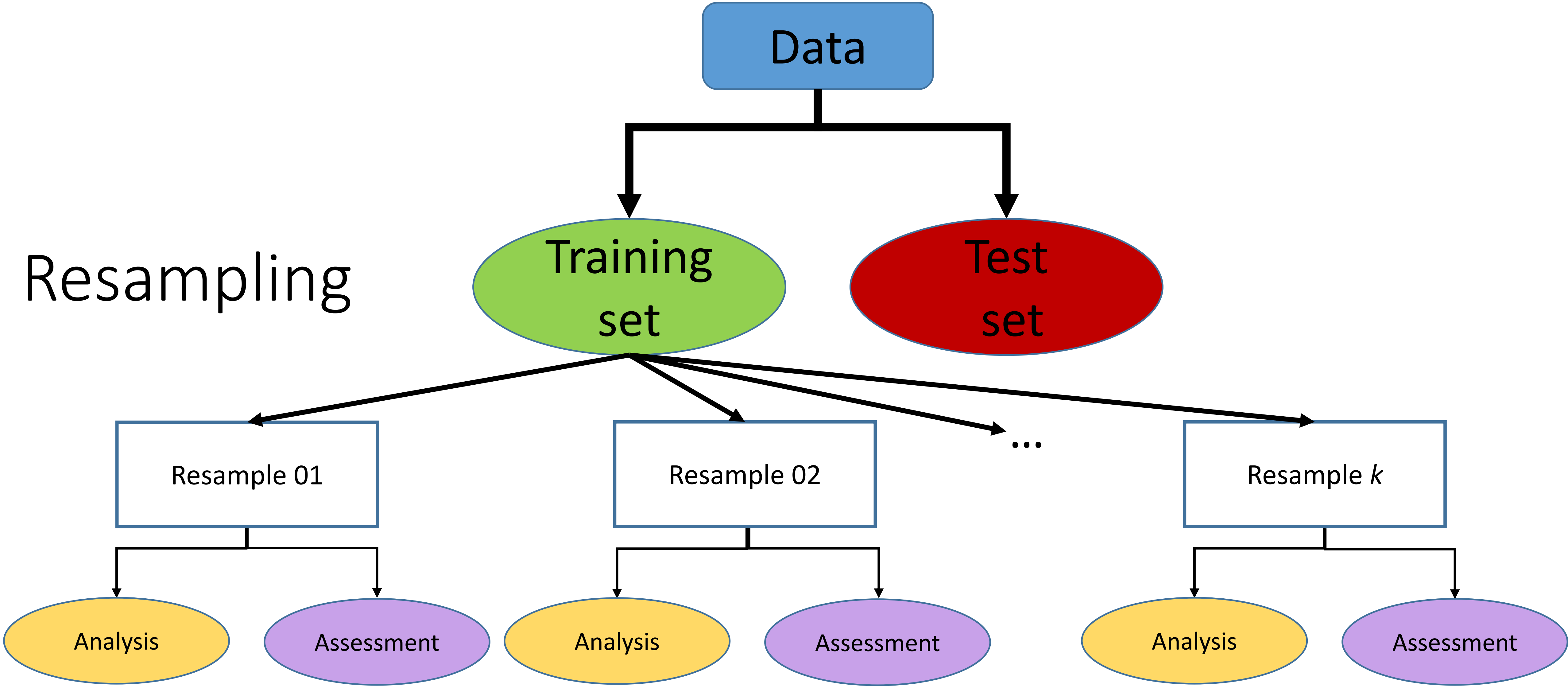
Training:Test::Analysis:Assessment

-OR-

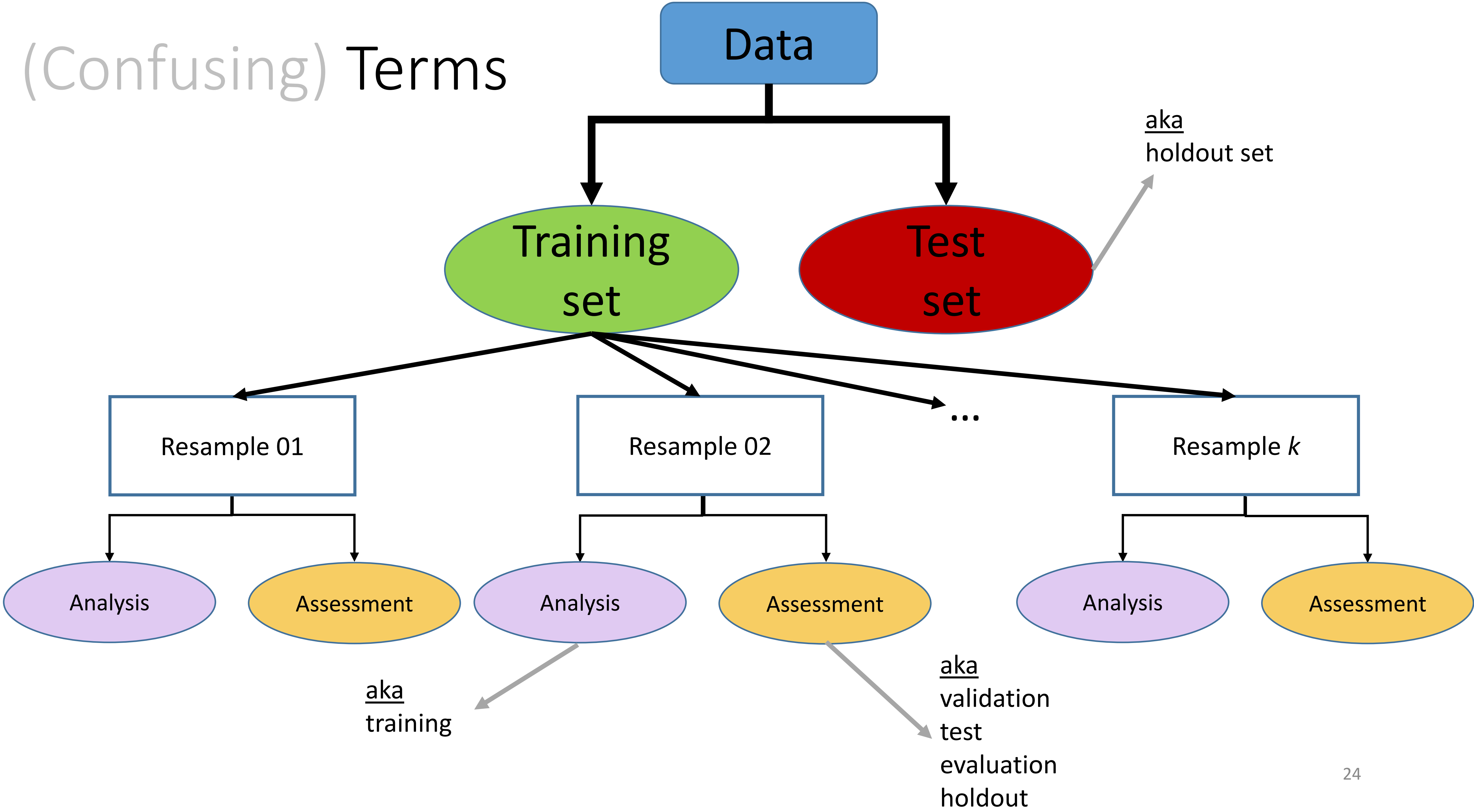
Analysis functions like the Training set

Assessment functions like the Test set

Resampling


Data
Training set
Test set
Resample 01
Resample 02
...
Resample *k*
Analysis
Assessment
Analysis
Assessment
Analysis
Assessment

(Confusing) Terms



Common Resampling Methods

- *k*-fold cross-validation
  - Probably the most common resampling method for model evaluation and model selection in applied ML
- Monte Carlo cross-validation
- Bootstrapping
- Leave one out cross validation (LOOCV)
- Others (not discussed here)
  - Rolling origin forecasting – for time series data
  - 632 and 632+ methods
  - Maximum dissimilarity sampling

k-fold cross-validation (*k*-fold CV)

- We randomly split the training data into *k* distinct samples ("folds") of (approximately) equal size

10-fold CV

- *k* = 10
- Within each fold, a random 10% (1/10) of training data are sampled for the assessment set
  - The 10% assessment sample is completely different for each fold
  - Each observation (row) serves in **one and only one assessment sample**
- The remaining 90% of the training data serve as the analysis set in the fold

10-fold CV

🟨 Assessment

🟪 Analysis

	Fold01	Fold02	Fold03	Fold04	Fold05	Fold06	Fold07	Fold09	Fold09	Fold10
01	🟨	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪
02	🟪	🟨	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪
03	🟪	🟪	🟨	🟪	🟪	🟪	🟪	🟪	🟪	🟪
04	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟪	🟪	🟪
05	🟪	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟪	🟪
06	🟪	🟪	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟪
07	🟪	🟪	🟪	🟪	🟪	🟪	🟨	🟪	🟪	🟪
08	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟨	🟪	🟪
09	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟨	🟪
10	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟨

k-fold CV

5-fold CV

- *k* = 5
- Within each fold, a random 20% (1/5) of training data are sampled for the assessment set
  - The 20% assessment sample is completely different for each fold
  - Each observation (row) serves in **one and only one assessment sample**
- The remaining 80% of the training data serve as the analysis set in the fold

5-fold CV

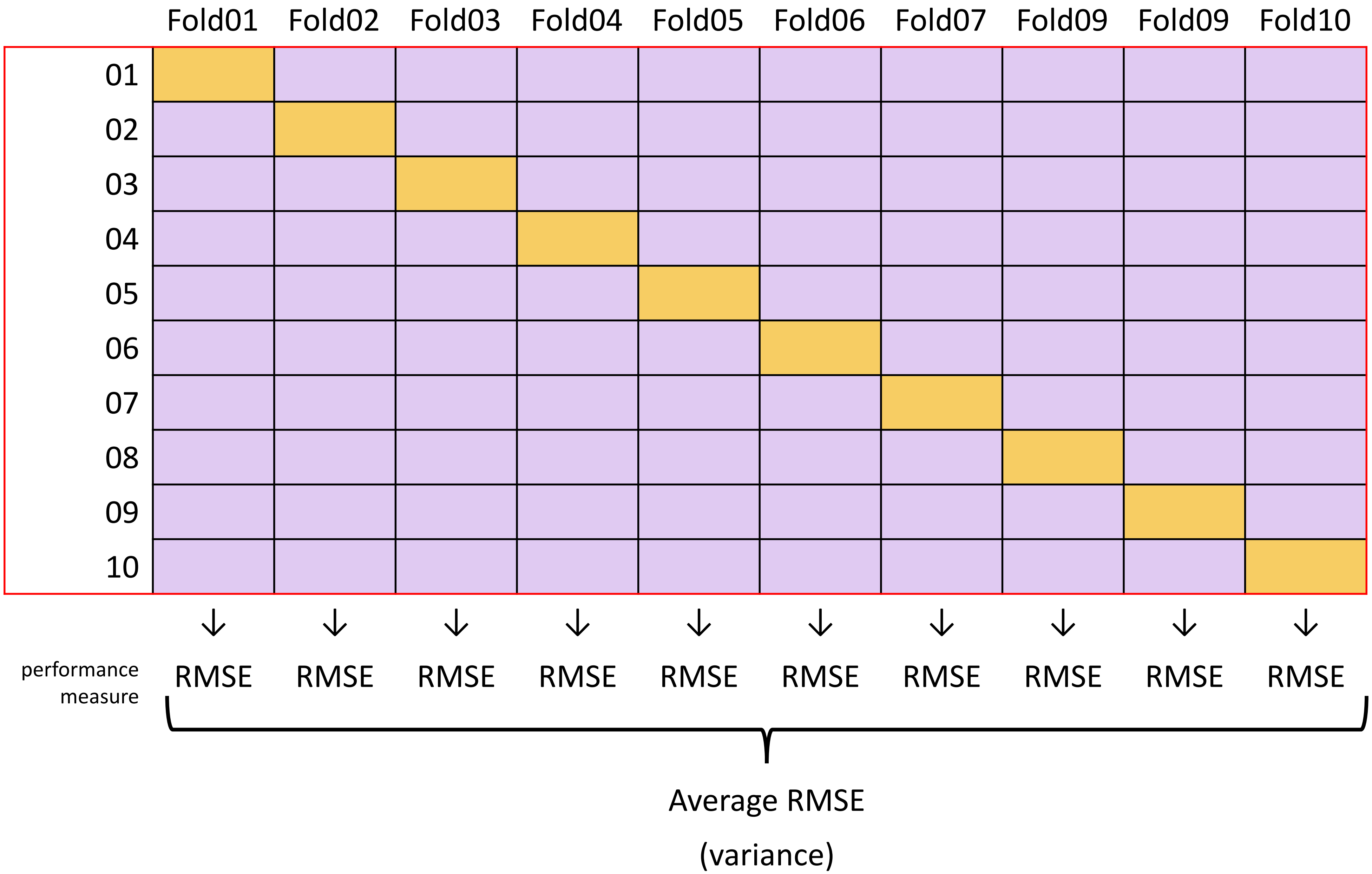
🟨 Assessment

🟪 Analysis

	Fold01	Fold02	Fold03	Fold04	Fold05
01	🟨	🟪	🟪	🟪	🟪
02	🟨	🟪	🟪	🟪	🟪
03	🟪	🟨	🟪	🟪	🟪
04	🟪	🟨	🟪	🟪	🟪
05	🟪	🟪	🟨	🟪	🟪
06	🟪	🟪	🟨	🟪	🟪
07	🟪	🟪	🟪	🟨	🟪
08	🟪	🟪	🟪	🟨	🟪
09	🟪	🟪	🟪	🟪	🟨
10	🟪	🟪	🟪	🟪	🟨

Results

- `Fold01`
  - We fit our model on the `Fold01` analysis set (leaving out the assessment set)
  - We apply our resulting model parameters to predict the assessment set
  - We get our performance measures (objective functions)
- We repeat this process until we've predicted all *k* assessment sets
- The final performance is the aggregate (*average)* performance measure across the *k* folds



	Fold01	Fold02	Fold03	Fold04	Fold05	Fold06	Fold07	Fold09	Fold09	Fold10
01	🟨	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪
02	🟪	🟨	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪
03	🟪	🟪	🟨	🟪	🟪	🟪	🟪	🟪	🟪	🟪
04	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟪	🟪	🟪
05	🟪	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟪	🟪
06	🟪	🟪	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟪
07	🟪	🟪	🟪	🟪	🟪	🟪	🟨	🟪	🟪	🟪
08	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟨	🟪	🟪
09	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟨	🟪
10	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟨
performance measure	RMSE	RMSE	RMSE	RMSE	RMSE	RMSE	RMSE	RMSE	RMSE	RMSE

Average RMSE

(variance)

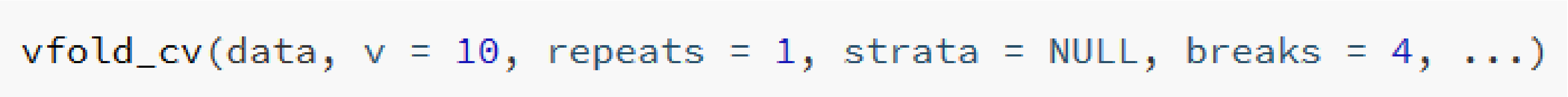
k-fold CV suggestions

- Larger values of *k*:
  - produce less bias (because the difference between a fold and the training set decreases)
  - more computationally intensive
- 10 folds is a good rule-of-thumb
  - Leave-one-out is the most extreme resampling technique
    - Use *n* - 1 to predict each row
  - 10-fold CV performed comparably to LOOCV (Molarino, 2005)

k-fold CV suggestions

- Has more variability compared to other resampling methods (bootstrapping)
- **Repeating** *k*-fold CV can improve the accuracy of the estimates while maintaining small bias (Molarino, 2005; Kim, 2009)
  - Helps reduce variability between folds; gives a more complete estimate of the overall between-fold variability (i.e., the variance distribution)
    - 10-fold CV repeated 5 times = 50 models/performance measures
    - Particularly useful for smaller data sets
    - For large training sets, variance and bias issues are less of a concern
  - Repeated CV is not equivalent to increasing the number of folds (e.g., 50-fold CV)

vfold_cv()



```
vfold_cv(data, v = 10, repeats = 1, strata = NULL, breaks = 4, ...)
```

data = your training set from training()

v = number of folds (default = 10)

repeats = number of repeats (default = 1)

strata = variable to conduct stratified sampling to create the folds

breaks = the number of bins desired to stratify a numeric stratification variable

vfold_cv()

```
set.seed(3000)
(cv_splits <- vfold_cv(math_train))
```

```
#  10-fold cross-validation
# A tibble: 10 x 2
   splits                          id
   <named list>                    <chr>
 1 <split [127.9K/14.2K]> Fold01
 2 <split [127.9K/14.2K]> Fold02
 3 <split [127.9K/14.2K]> Fold03
 4 <split [127.9K/14.2K]> Fold04
 5 <split [127.9K/14.2K]> Fold05
 6 <split [127.9K/14.2K]> Fold06
 7 <split [127.9K/14.2K]> Fold07
 8 <split [127.9K/14.2K]> Fold08
 9 <split [127.9K/14.2K]> Fold09
10 <split [127.9K/14.2K]> Fold10
```

vfold_cv()

```
cv_splits$splits[[1]]
<Analysis/Assess/Total>
<127863/14207/142070>

cv_splits$splits[[1]] %>%
   analysis() %>%
   nrow()
[1] 127863

cv_splits$splits[[1]] %>%
  assessment() %>%
  nrow()
[1] 14207
```

```
cv_splits$splits[[1]]
<Analysis/Assess/Total>
<127863/14207/142070>
```

```
cv_splits$splits[[1]] %>%
  assessment()
```

```
# A tibble: 14,207 x 40
      id gndr  ethnic_cd attnd_dist_inst~ attnd_schl_inst~ enrl_grd calc_admn_cd
   <dbl> <chr> <chr>                <dbl>            <dbl>    <dbl> <lgl>
 1    37 F     W                     2042              387        8 NA
 2    47 M     M                     2142             1330        8 NA
 3    72 M     W                     2057              480        7 NA
 4    96 F     A                     2041              380        8 NA
 5   109 M     W                     2090              593        7 NA
 6   146 M     W                     1926               97        7 NA
 7   175 M     W                     2082              528        8 NA
 8   189 F     W                     2087             4555        7 NA
 9   196 M     W                     2082              506        8 NA
10   206 M     B                     1970              224        7 NA
# ... with 14,197 more rows, and 33 more variables:
```

Monte Carlo Cross-Validation

- For each split, a random sample (without replacement) is taken with a specified proportion going into the analysis set and the rest going to the assessment set
- The splitting procedure is conducted a specified number times
  - The number of splits must be large enough have adequate precision
- Like *k*-fold CV, a model is created on the analysis set and the assessment set is used to evaluate the model, and the average of the results across resamples are used to estimate future performance
- As opposed to *k*-fold CV, MC CV produces resamples that are likely to contain overlap

10-fold CV

🟨 Assessment

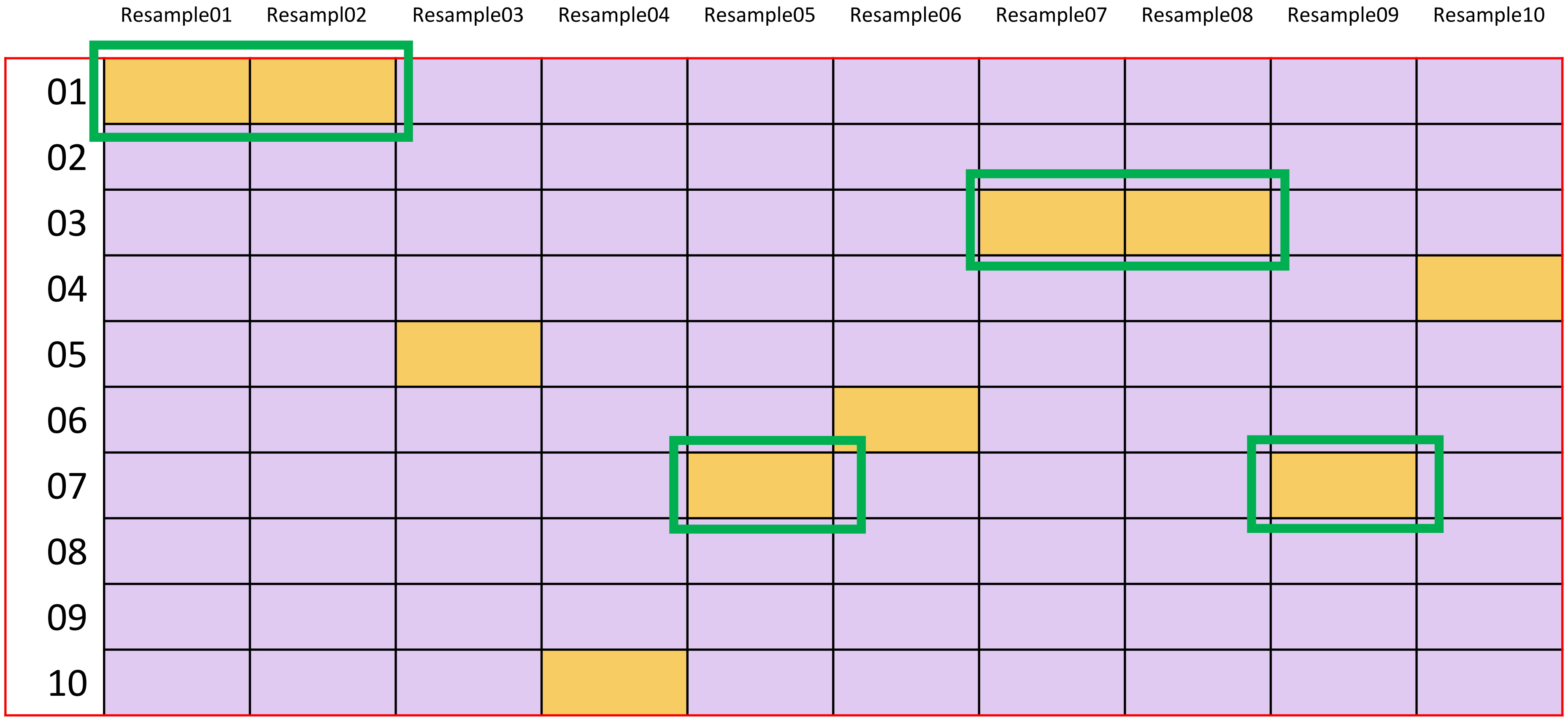
🟪 Analysis

	Fold01	Fold02	Fold03	Fold04	Fold05	Fold06	Fold07	Fold09	Fold09	Fold10
01	🟨	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪
02	🟪	🟨	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪
03	🟪	🟪	🟨	🟪	🟪	🟪	🟪	🟪	🟪	🟪
04	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟪	🟪	🟪
05	🟪	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟪	🟪
06	🟪	🟪	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟪
07	🟪	🟪	🟪	🟪	🟪	🟪	🟨	🟪	🟪	🟪
08	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟨	🟪	🟪
09	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟨	🟪
10	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟨

Monte Carlo CV (10 times)

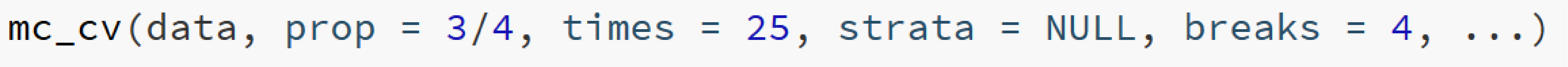
🟨 Assessment

🟪 Analysis



	Resample01	Resampl02	Resample03	Resample04	Resample05	Resample06	Resample07	Resample08	Resample09	Resample10
01	🟨	🟨	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪
02	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪
03	🟪	🟪	🟪	🟪	🟪	🟪	🟨	🟨	🟪	🟪
04	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟨
05	🟪	🟪	🟨	🟪	🟪	🟪	🟪	🟪	🟪	🟪
06	🟪	🟪	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟪
07	🟪	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟨	🟪
08	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪
09	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪	🟪
10	🟪	🟪	🟪	🟨	🟪	🟪	🟪	🟪	🟪	🟪

mc_cv()



```
mc_cv(data, prop = 3/4, times = 25, strata = NULL, breaks = 4, ...)
```

`data` = your training set

`prop` = proportion going to the analysis set (default = .75)

`times` = number of times to repeat the sample (default = 25)

`strata` = variable to conduct stratified sampling to create the folds

`breaks` = the number of bins desired to stratify a numeric stratification variable (default = 4)

mc_cv()

```
(mc_splits <- mc_cv(math_train))
```

```
# # Monte Carlo cross-validation (0.75/0.25) with 25 resamples
# A tibble: 25 x 2
   splits                    id
   <list>                    <chr>
 1 <split [106.6K/35.5K]> Resample01
 2 <split [106.6K/35.5K]> Resample02
 3 <split [106.6K/35.5K]> Resample03
 4 <split [106.6K/35.5K]> Resample04
 5 <split [106.6K/35.5K]> Resample05
 6 <split [106.6K/35.5K]> Resample06
 7 <split [106.6K/35.5K]> Resample07
 8 <split [106.6K/35.5K]> Resample08
 9 <split [106.6K/35.5K]> Resample09
10 <split [106.6K/35.5K]> Resample10
# ... with 15 more rows
```

mc_cv()

```
nrow(math_train)
[1] 142070
```

```
mc_splits$splits[[1]]
<106553/35517/142070>
```

```
mc_splits$splits[[12]]
<106553/35517/142070>
```

```
mc_splits$splits[[25]]
<106553/35517/142070>
```

```
analysis(mc_splits$splits[[1]]) %>% nrow() / nrow(mc_splits$splits[[1]]$data)
[1] 0.7500035
```

mc_cv()

```
nrow(math_train)
[1] 142070

mc_splits$splits[[1]]
<106553/35517/142070>

mc_splits$splits[[12]]
<106553/35517/142070>

mc_splits$splits[[25]]
<106553/35517/142070>

analysis(mc_splits$splits[[1]]) %>% nrow() / nrow(mc_splits$splits[[1]]$data)
[1] 0.7500035
```

bootstrapping

- A bootstrap sample is a **simple random sample** that is the **same size as the training set** where the data are **sampled with replacement**
  - So after a row is selected for inclusion in the subset, it's still available for further selection
- Each bootstrap sample is likely to contain duplicate values
  - Analysis set
    - On average, 63.21% of the original sample ends up in a bootstrap sample
  - Assessment set
    - Those rows not selected in a bootstrap sample are considered **out-of-bag** (OOB)

Times sampled:	0	1	2	3
	□	░	▒	■

Assessment

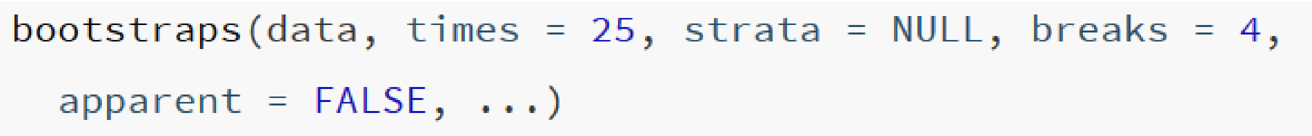
Analysis

	B01	B02	B03	B04	B05	B06	B07	B09	B09	B10
01	░	□	▒	░	░	□	░	░	□	□
02	▒	░	░	░	░	□	▒	■	□	□
03	□	░	□	▒	□	░	░	■	□	░
04	▒	░	■	░	□	░	▒	□	□	░
05	□	░	▒	▒	░	░	□	▒	□	░
06	■	░	□	□	░	▒	□	░	▒	□
07	□	▒	□	░	░	▒	░	░	□	▒
08	░	▒	░	□	▒	░	□	░	□	■
09	░	░	░	□	░	■	░	░	▒	□
10	░	□	▒	░	▒	░	▒	□	░	□

Bootstrap vs K-fold CV

- K-fold CV tends to have less bias and more variance
- bootstrapping tends to have more bias but less variance
- bootstrap has more bias because of replacement (similar to $k = 2$)
  - This is problematic when the training set is small, and less so as the sample increases ($n \geq 1{,}000$)

bootstraps()



```
bootstraps(data, times = 25, strata = NULL, breaks = 4,
  apparent = FALSE, ...)
```

`data` = your training set

`times` = number of bootstrap samples (default = 25)

`strata` = variable to conduct stratified sampling to create the folds

`breaks` = the number of bins desired to stratify a numeric stratification variable

`apparent` = enables the option of an additional resample where the analysis and assessment data sets are the same as the original data set. This can be required for some types of analysis of the bootstrap results.

bootstraps()

> (boot_splits <- bootstraps(math_train))

```
# Bootstrap sampling
# A tibble: 25 x 2
   splits                      id
   <list>                      <chr>
 1 <split [142.1K/52.1K]> Bootstrap01
 2 <split [142.1K/52.2K]> Bootstrap02
 3 <split [142.1K/52.2K]> Bootstrap03
 4 <split [142.1K/52.4K]> Bootstrap04
 5 <split [142.1K/52.3K]> Bootstrap05
 6 <split [142.1K/52.2K]> Bootstrap06
 7 <split [142.1K/52.2K]> Bootstrap07
 8 <split [142.1K/52.5K]> Bootstrap08
 9 <split [142.1K/52.3K]> Bootstrap09
10 <split [142.1K/52.4K]> Bootstrap10
# ... with 15 more rows
```

bootstraps()

```
nrow(math_train)
[1] 142070
```

```
boot_splits$splits[[1]]
<Analysis/Assess/Total>
<142070/52415/142070>
```

```
boot_splits$splits[[12]]
<142070/52447/142070>
```

```
boot_splits$splits[[25]]
<142070/52149/142070>
```

Results

- `B01`
  - We fit our model on the `B01` analysis set (leaving out the assessment set)
  - We apply our resulting model parameters to predict the assessment set
  - We get our performance measures (loss functions)
- We repeat this process until we've predicted all *B* assessment sets
- The final performance is the *average* performance measure across the *B* sets

Leave-one-out (LOO) cross-validation

- Uses one data point in the original set as the assessment data and all other data points as the analysis set
- A LOO resampling set has as many resamples as rows in the original data set
- LOO is computationally excessive unless you have extremely small sample
- Generally may not have good statistical properties

loo_cv()

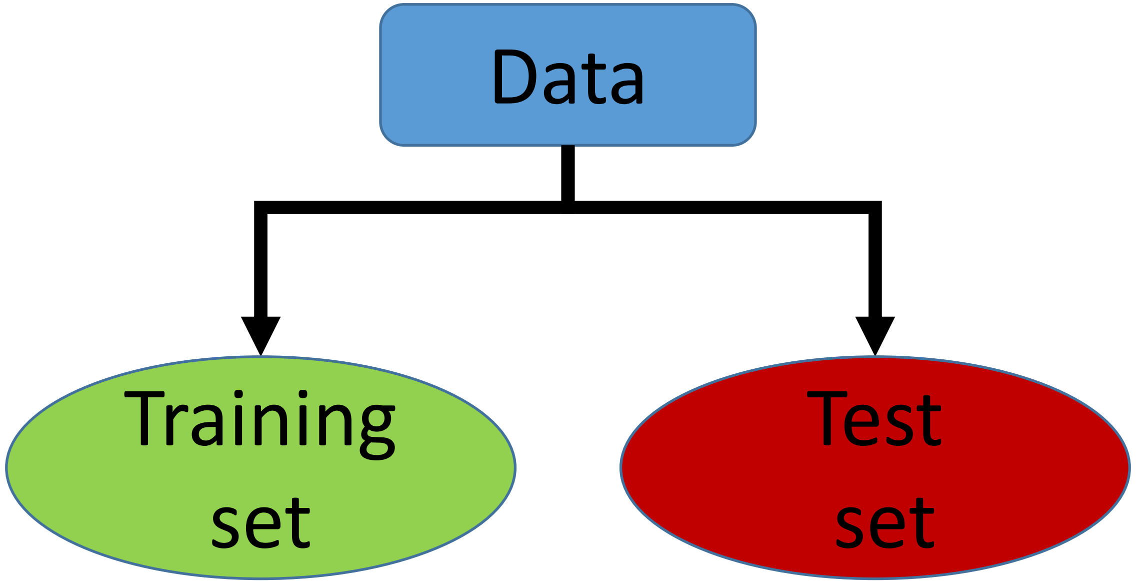
```
loo_cv(data, ...)
```

```
> (loo_splits <- loo_cv(sample_n(math_train, 10000)))
```

```
# Leave-one-out cross-validation
# A tibble: 10,000 x 2
   splits            id
   <named list>      <chr>
 1 <split [10K/1]> Resample1
 2 <split [10K/1]> Resample2
 3 <split [10K/1]> Resample3
 4 <split [10K/1]> Resample4
 5 <split [10K/1]> Resample5
 6 <split [10K/1]> Resample6
 7 <split [10K/1]> Resample7
 8 <split [10K/1]> Resample8
 9 <split [10K/1]> Resample9
10 <split [10K/1]> Resample10
# ... with 9,990 more rows
```

```
> loo_splits$splits[[1]]
<Analysis/Assess/Total>
<9999/1/10000>

> loo_splits$splits[[12]]
<Analysis/Assess/Total>
<9999/1/10000>

> loo_splits$splits[[101]]
<Analysis/Assess/Total>
<9999/1/10000>
```

Quick recap

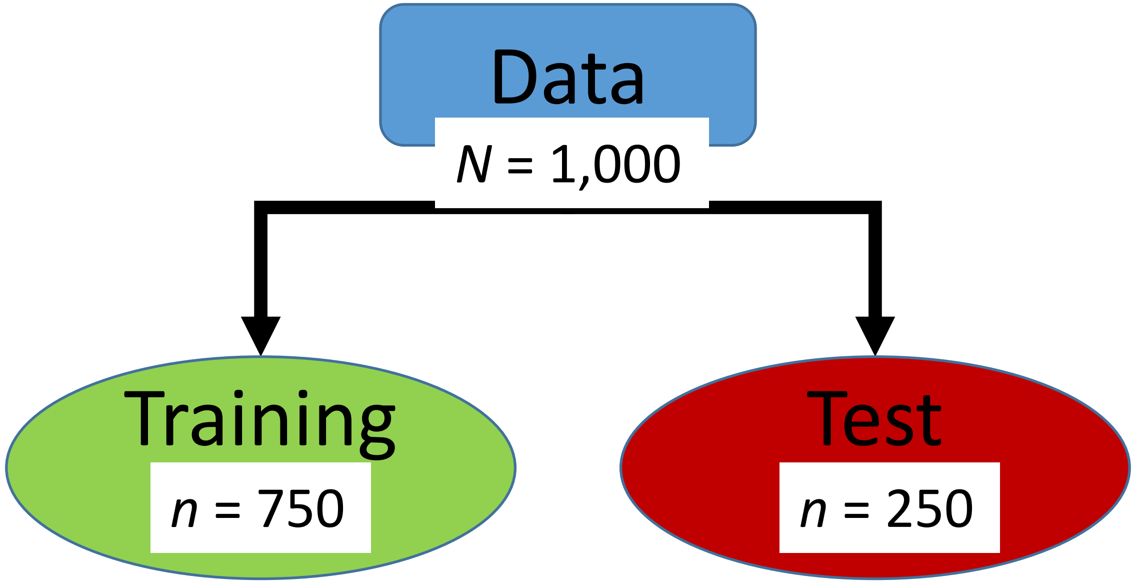


Data

Training set

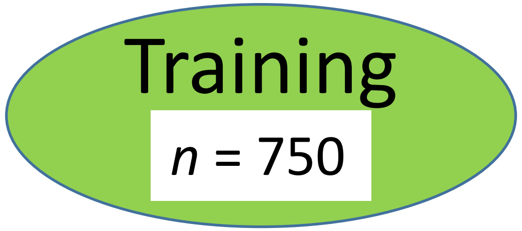
Test set

```
math_split <- initial_split(math)

math_train <- training(math_split)
math_test  <- testing(math_split)
```



```
math_split <- initial_split(math)

math_train <- training(math_split)
math_test  <- testing(math_split)
```

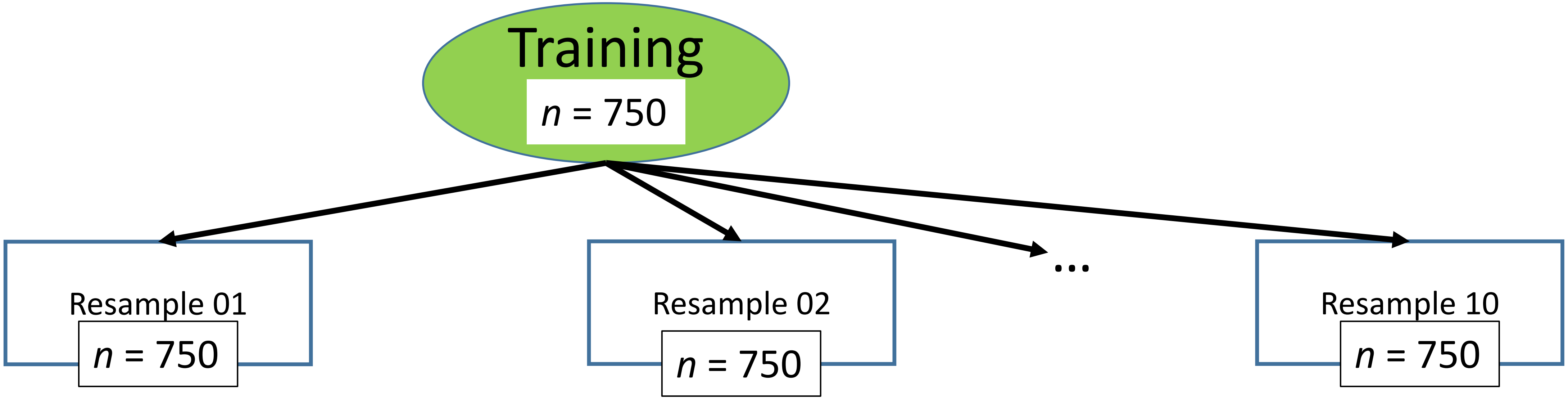
Resampling



Training

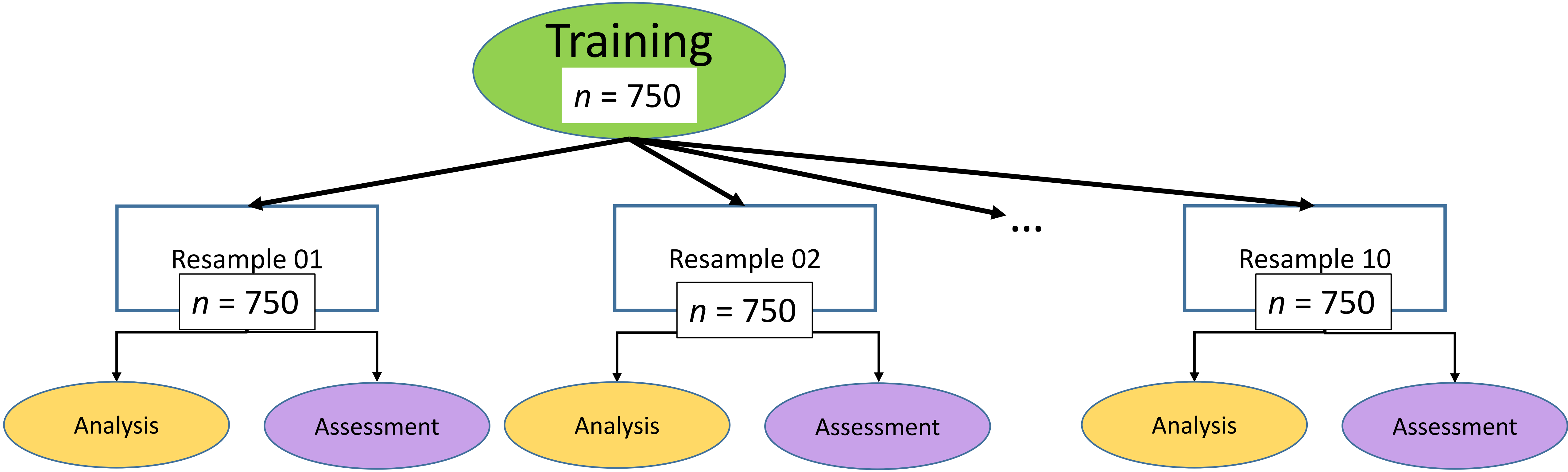
n = 750

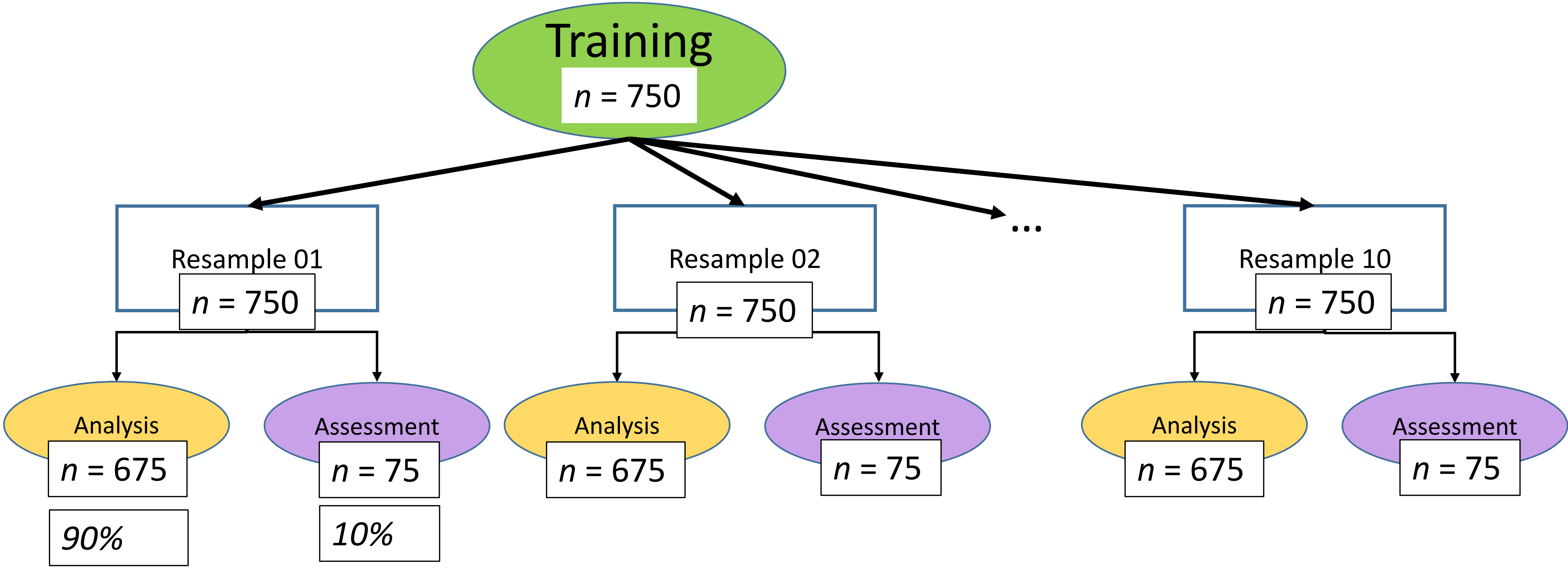
10-fold CV



```
math_splits <- vfold_cv(math_train)
```

10-fold CV so 1/10th of Resample goes to each assessment set to get unique assessment sets across 10 resamples




Training
n = 750
Resample 01
n = 750
Resample 02
n = 750
…
Resample 10
n = 750
Analysis
n = 675
90%
Assessment
n = 75
10%
Analysis
n = 675
Assessment
n = 75
Analysis
n = 675
Assessment
n = 75

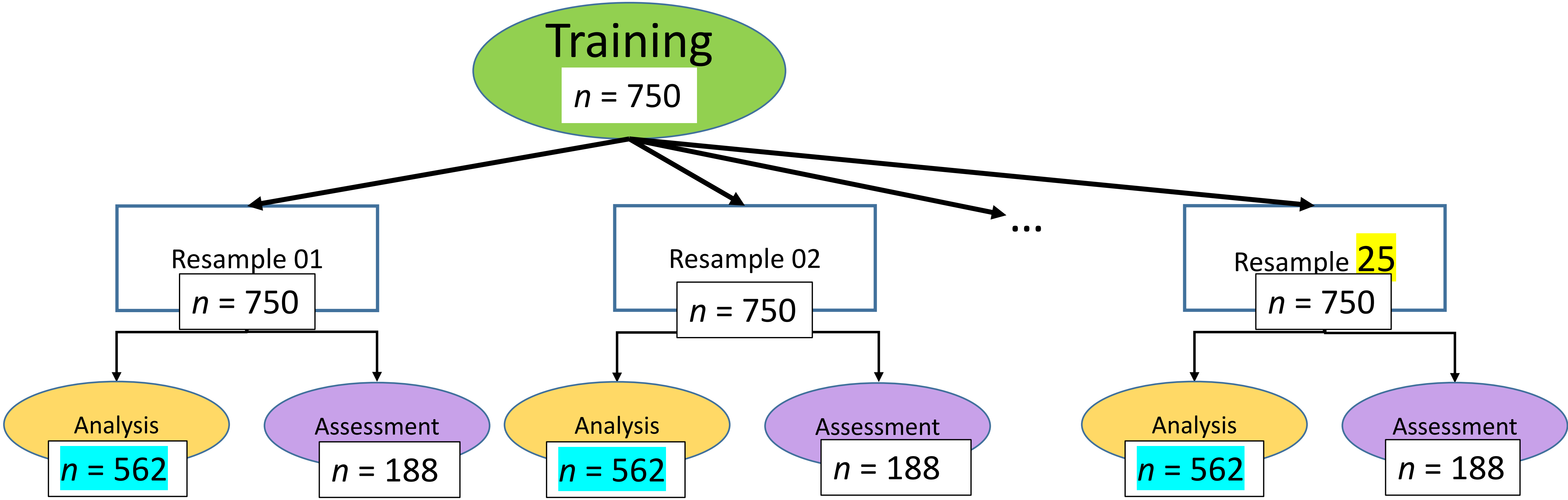
vfold_cv()

```
math_splits$splits[[1]] %>%
  analysis()

math_splits$splits[[1]] %>%
  assessment()
```

Monte Carlo Cross-Validation

- For each split, a random sample (without replacement) is taken with a specified proportion going into the analysis set and the rest going to the assessment set
- As opposed to *k*-fold CV, MC CV produces resamples that are likely to contain overlap

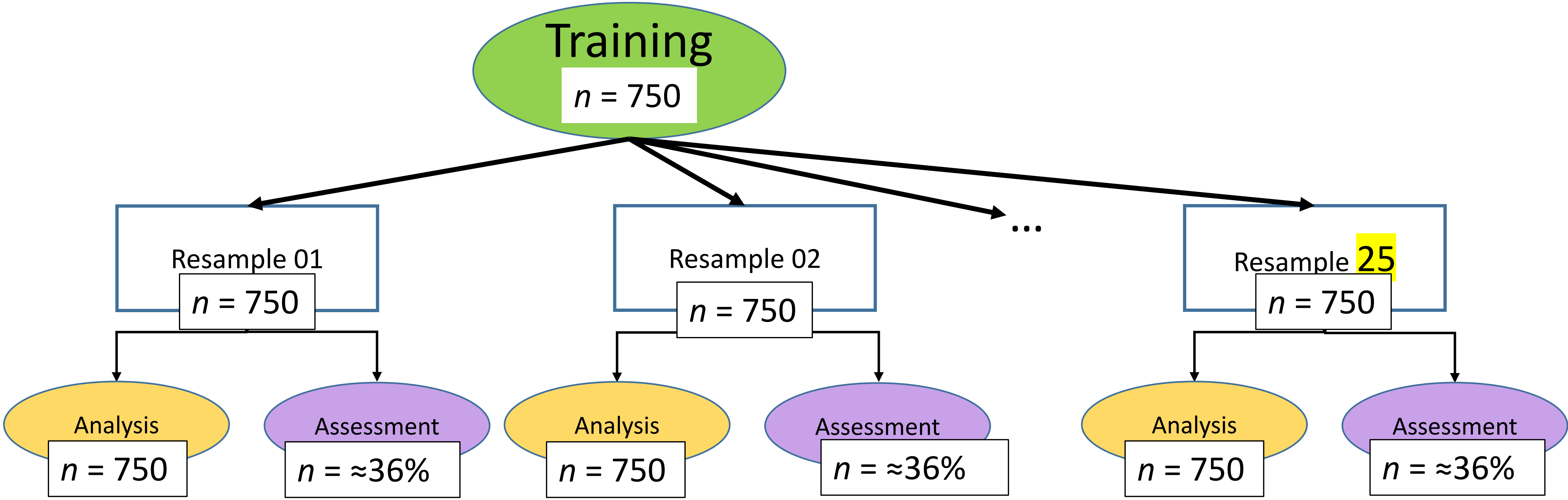
```
mc_splits <- mc_cv(math_train,
                   prop = .75, #default
                   times = 25) #default
```



bootstrapping

- A bootstrap sample is a **simple random sample** that is the **same size as the training set** where the data are sampled **with replacement**
  - So after a row is selected for inclusion in the assessment, it’s still available for further selection
- Each bootstrap sample is likely to contain duplicate values
  - Analysis set
    - On average, 63.21% of the original sample ends up in a bootstrap sample
  - Assessment set
    - Those rows not selected in a bootstrap sample are considered **out-of-bag** (OOB)

```
mc_splits <- bootstraps(math_train,
                        times = 25) #default
```



Results

- `Fold01`
  - We fit our model on the `Fold01` analysis set (leaving out the assessment set)
  - We apply our resulting model parameters to predict the assessment set
  - We get our performance measures (objective functions)
- We repeat this process until we've predicted all *k* assessment sets
- The final performance is the *average* performance measure across the *k* folds

Resampling considerations

- Small sample size: repeated 10-fold CV
  - bias-variance properties are good
  - low computational cost
- Large sample size: 10-fold CV
  - less difference between methods
  - computationally efficient

Next time

- Lab 1
- Readings

Lab 1

Resampling notes

- *k*-fold CV more variability compared to other resampling methods (bootstrapping)
  - **Repeating** *k*-fold CV can improve the accuracy of the estimates while maintaining small bias (Molarino, 2005; Kim, 2009)
  - Helps reduce variability between folds10-fold CV repeated 5 times = 50 models/performance measures
    - Particularly useful for smaller data sets
    - For large training sets, variance and bias issues are less of a concern
- Bootstrap tends to have less variability in the error measure compared to *k*-fold CV
- But because of replacement, bootstrap has more bias (similar to *k* = 2)
  - This is problematic when the training set is small, and less so as the sample increases (*n* ≥ 1,000)